

7,7'-(Carbonyldiimino)bis[4-hydroxy-2-naphthalenesulfonic acid]
134-47-4 | DTXSID7059642

Model Performance

Model	Data
-------	------

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 2.69

Global applicability domain: Outside

Local applicability domain index: 1.45e-01

Confidence level: 8.13e-01

Nearest Neighbors from the Training Set

Image not found

7,7'-(Carbonyldiimino)bis[4-hydroxy-2-naphthalenesulfonic acid]

Measured: 1.82
Predicted: 2.69

Image not found

4-Amino-5-hydroxy-2,7-naphthalenedisulfonic acid monosodium salt

Measured: 2.88
Predicted: 2.48

Image not found

Docusate sodium
Measured: 9.33
Predicted: 8.95

Image not found

7-Amino-4-hydroxynaphthalene-2-sulfonic acid

Measured: 2.40
Predicted: 4.77